Atomic final-state effects in nuclear transitions

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The interaction of a nuclear gamma radiation with the atomic electron cloud gives rise to a phase shift in the nuclear electromagnetic transition amplitude. The resulting interference parameters $\xi(\pi L)$ are of significance to the analysis of time-reversal experiments. We calculate these parameters for $E1$, $E2$, $E3$, $M1$, and $M2$ gamma transitions in a number of nuclei. We also discuss the implication of these results for simultaneous parity- and time-reversal-violating experiments.

Photons emitted in a nuclear transition may interact with the atomic electron cloud. In particular, elastic-scattering processes will interfere with direct photon emission resulting in a modification of the nuclear electromagnetic transition amplitudes [1,2] which become, in general, complex. A knowledge of such effects is necessary for the interpretation of experiments involving the measurement of time-(T) or simultaneous parity- and time- (PT) reversal-violating nuclear gamma-ray distributions [3]. Here one seeks to measure a relative phase between the transition matrix elements [4] $\gamma(\pi L,\psi_i\rightarrow\psi_f)$ of two competing electromagnetic multipoles (πL and $\pi' L'$), as expressed by the mixing ratio

$$\delta_{LL'}=\gamma(\pi L,\psi_i\rightarrow\psi_f)/\gamma(\pi' L',\psi_i\rightarrow\psi_f)$$
$$=|\delta_{LL'}|e^{i\eta_{LL'}} . \quad (1)$$

For a T-conserving nuclear Hamiltonian one may always adopt a suitable phase convention for the initial and final nuclear states $\psi_{i,f}$ such that the transition amplitudes are relatively real and thus $\eta_{LL'}=\eta(\pi L)-\eta(\pi' L')=0$ or π. A departure of $\eta_{LL'}$ from these values would then be the signature of a T- or PT-violating component in the nuclear interaction. However, this conclusion is not unambiguous since the mixing ratio can also acquire an additional phase through the "final-state" interaction of the radiated photon with the surrounding atomic electrons as indicated above. The relevant processes are shown in Fig. 1. Figure 1(a) represents the amplitude $\gamma(\pi L,\psi_i\rightarrow\psi_f)$ for the direct emission of a photon. Figures 1(b) and (c) show the leading-order elastic-scattering processes of this photon with electrons in atomic bound states "0" possessing energies E_0. The combined amplitude for these latter diagrams can be written

$$[\rho(\pi L)+i\xi(\pi L)]\gamma(\pi L,\psi_i\rightarrow\psi_f) ,$$

where the real part $\rho(\pi L)$ is of little interest here. The total transition amplitude therefore acquires, through the final-state interaction, an additional phase $\xi(\pi L)$ of order α which is also present in the observed multipole mixing ratio

$$\delta_{LL'}=|\delta_{LL'}|e^{i(\eta_{LL'}+\xi_{LL'})} , \quad (2)$$

where $\xi_{LL'}=\xi(\pi L)-\xi(\pi' L')$. Experimentally, the spurious electromagnetic phase ξ cannot be distinguished from the genuine T-violating nuclear phase η and therefore a theoretical determination of these final-state effects is essential. We have extended the previous work of Davis *et al.* [1], henceforth referred to as I, to include additional $M2$ and $E3$ gamma-ray multipolarities. We also consider gamma-ray energies, ω, greater than the electron-positron pair-creation threshold ($\omega\geq 2m_e$) which were not included in I. By calculating positron solutions in the Coulomb field of the nucleus and then charge conjugating to yield the negative-energy electron wave functions ($E<-m_e$), we are able to retain the Green's-function formalism outlined in the Appendix of I without modification.

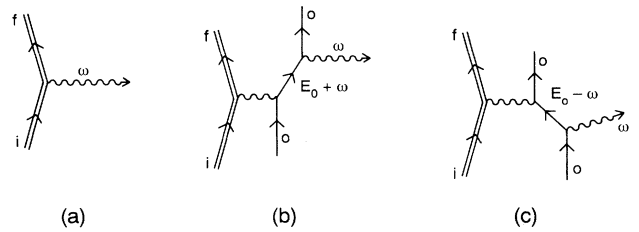

FIG. 1. The Feynman graphs describing the amplitude for photon emission in a nuclear transition. The wavy lines represent the emitted and virtual photon, the straight lines represent the bound and virtual electrons, and the double lines the nucleus.

In I, the relationship of the $E_0+\omega$ intermediate-energy electron energy diagram, Fig. 1(b), to the well-known processes of internal conversion and the photoeffect was used as a check of the numerical work. For gamma-ray energies above the pair-creation threshold, the $E_0-\omega$ intermediate-energy electron diagram, Fig. 1(c), may be related to analogous processes thus checking the present calculations and giving us, at the same time, the capability to describe other processes. The two effects in question correspond to a pair creation by the nuclear gamma ray in which the electron occupies a bound atomic state, the so-called conversion with the emission of monoenergetic positrons, and to the annihilation of a positron on a bound atomic electron with the creation of a single photon.

The former process is difficult to observe since it requires the presence of an electron vacancy at the time of the nuclear transition. We made a comparison with theoretical formulas for this type of internal conversion, calculated in the Born limit assuming $Z\alpha \ll 1$ [5]. (The expressions of Ref. [5] omit factors m_e/ω.) We were able to reproduce these formulas with the given approximations although a full calculation yields conversion coefficients which are somewhat smaller. (See also the results of a more realistic calculation [6].)

The second process, the one-photon positron annihilation, was proposed in 1933 by Fermi and Uhlenbeck [7] and is treated theoretically by Heitler [8] for the case $\alpha Z \ll 1$. [Again, the corresponding Eq. (33.16) in Ref. [5] contains an error.] For light nuclei we obtained results in agreement with the approximate formula [8]. However, for heavier nuclei, the effects of the atomic binding and the screened nuclear Coulomb field contrive to reduce to the cross section for this process in a qualitatively similar manner to the analogous photelectric effect.

Finally, in Ref. [2] the scattering phase was approximated by the nonrelativistic Thomson screening. Even at gamma-ray energies of 2 MeV in heavy nuclei we find that, numerically, this approximation remains good to a factor of 2, despite the simplicity of the expression.

In Fig. 2 we plot the atomic final-state phase shifts for five different multipolarities of gamma transitions with energies between 0.2 and 2 MeV. These are given for $Z=50$, 70, and 90. The solid and dashed lines correspond to the conversion and scattering phases, respec-

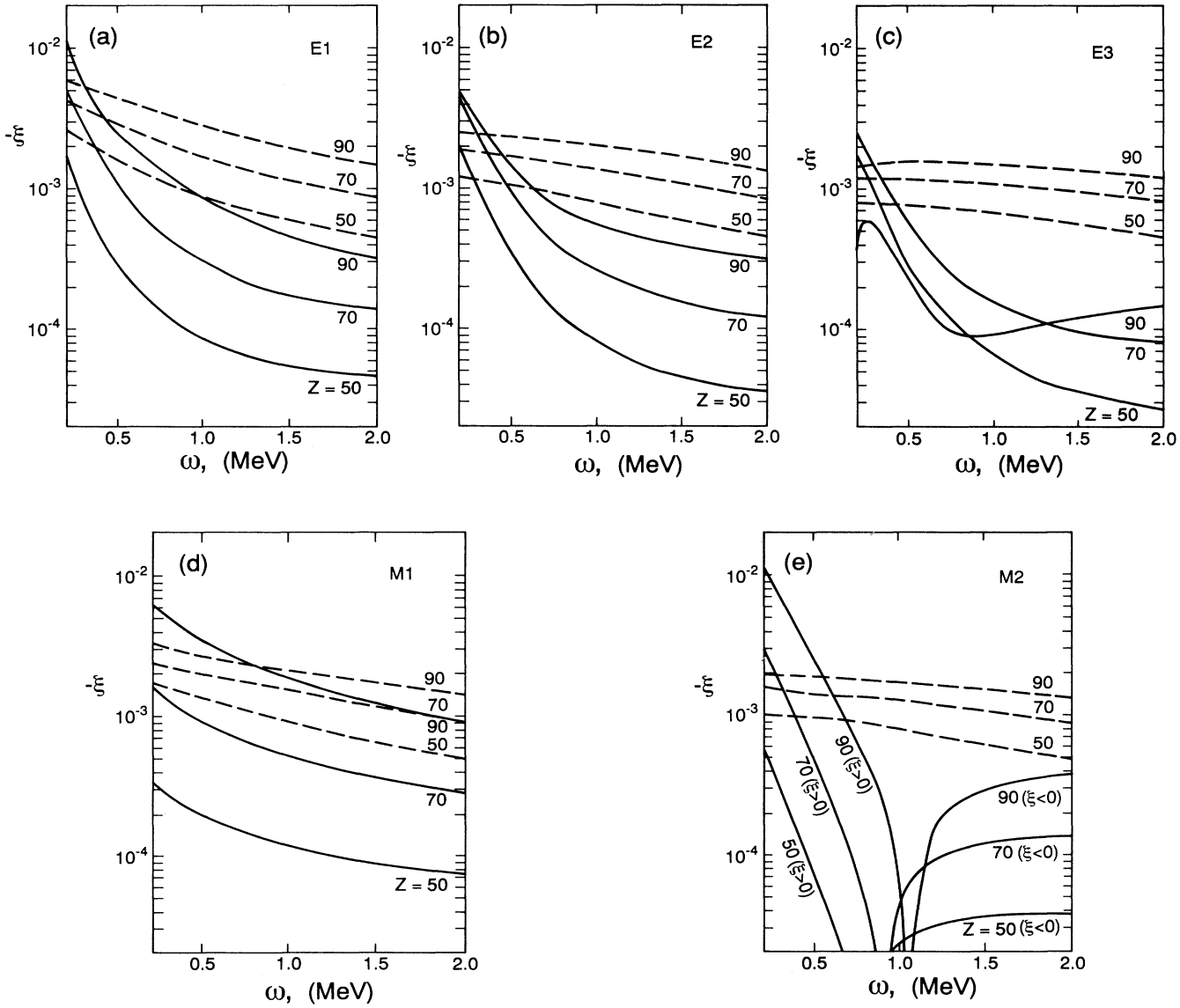

FIG. 2. The atomic final-state phase $\xi(\pi L)$ for gamma-ray energies between 0.2 and 2 MeV in nuclei of atomic number $Z=50$, 70, and 90. Transitions of multipolarities $\pi L = E1$, $E2$, $E3$, $M1$, and $M2$ are represented in (a)–(e) respectively. The solid lines give the conversion phases while the dashed lines give the scattering phases. Note that the $M2$ conversion phases are positive in the lower-energy region.

tively (as defined in I). The total phase shift for a given multipolarity is then given by the sum of these two contributions.

These diagrams are given for orientation purposes. In practice, a more detailed calculation for each transition is necessary. (Particularly so, since, at higher energies, the more dominant scattering phases tend toward similar values with little dependence upon multipolarity.) Therefore, in Table I we present the atomic final-state phase shifts for transitions in several nuclei which are of relevance to T- and PT-symmetry-violating experiments. These include the contributions from all bound atomic shells. The combined conversion and scattering phase shifts are given separately for each multipolarity. The uncertainty in these values is estimated to be about 2%. Note that it is the difference $\xi_{LL'}=\xi(\pi L)-\xi(\pi' L')$ between the phase shifts of two competing gamma-ray multipoles that occurs in the experimentally observed mixing ratio Eq. (2). The relative uncertainty in this difference can be somewhat greater.

Let us now apply our results to a particular case; namely, a measurement of the extent of PT-violating gamma-ray correlations in the decay of the isomeric 8^- state in ^{180}Hf [9]. From Ref. [10] it follows that the ratio of the PT-violating imaginary part to the P-violating real part of the "irregular" $\overline{E2}$, $M2$ mixing ratio ε_{22} is given as

$$\frac{\mathrm{Im}\varepsilon_{22}}{\mathrm{Re}\varepsilon_{22}}=[\xi(\overline{E2})-\xi(E3)]+\mathrm{Im}\frac{\langle a_1|V_{PT}|a_0\rangle}{\langle a_1|V_P|a_0\rangle}\ , \qquad (3)$$

where we have adopted a simple two-level mixing scenario for simplicity and $|a_0\rangle$, $|a_1\rangle$ represent the 8^-, 8^+ states, respectively. The presence of the $E3$ rather than the $M2$ final-state phase in this expression arises from the fact that the experimental PT-violating correlation in question is sensitive to $\overline{E2}$, $E3$ rather than $\overline{E2}$, $M2$ interference terms. Equation (3) shows that the significance of atomic final-state phases in PT-violation experiments depends on their magnitude relative to the ratio of PT- to P-violating nuclear matrix elements. The results of the ^{180}Hf experiment [9] indicate that $|\mathrm{Im}\varepsilon_{22}/\mathrm{Re}\varepsilon_{22}|<1.7$, so that the atomic final-state phase, which we calculate to be $\xi(\overline{E2})-\xi(E3)=-9\times10^{-4}$, is negligible.

In Ref. [10] we found that the ratio of PT- to P-violating matrix elements compatible with the upper limit of the neutron dipole moment is $\sim7\times10^{-4}$. Thus, a genuine PT-violating gamma-ray distribution in ^{180}Hf is likely to be masked by the atomic final-state effects even before a sensitivity at the level presently attained by the neutron electric dipole moment is reached. On the other hand, with the estimated uncertainty in our results it should be possible to reliably subtract the final-state phase to obtain the PT to P ratio down to the level of $\sim10^{-4}$. Such a measurement would set a limit on PT nonconservation, at least in the most favorable case of the isovector pion-exchange interaction, [11] an order of magnitude lower than that derived from the neutron electric dipole moment.

The restrictions may be somewhat relaxed by focusing experimental attention upon gamma radiations of higher energy, since, for these, the final-state phases are reduced. For example, in Ref. [10] we discussed the merits of a similar experiment performed upon the 1189-keV gamma ray in ^{182}W. This transition is associated with atomic final-state phases of only

$$\xi(E1)-\xi(\overline{E2})=-3.0\times10^{-4}$$

TABLE I. The atomic final-state phases $\xi(\pi L)$ for some gamma transitions in candidate nuclei for PT- (upper half) and T- (lower half) symmetry-violation tests.

Nucleus	E_γ (keV)	Atomic final-state phase $\xi(\pi L)$		
$^{157}_{64}$Gd	64	-3.99×10^{-2} ($E1$)	-4.06×10^{-3} ($\overline{M1}$)	-1.50×10^{-2} ($\overline{E2}$)
$^{169}_{69}$Tm	198	-4.04×10^{-3} ($M1$)	-6.43×10^{-3} ($E2$)	-9.79×10^{-3} ($\overline{E1}$)
	177	-4.22×10^{-3} ($M1$)	-7.31×10^{-3} ($E2$)	-1.12×10^{-2} ($\overline{E1}$)
$^{175}_{71}$Lu	354	-5.66×10^{-3} ($E1$)	-3.45×10^{-3} ($\overline{M1}$)	-3.58×10^{-3} ($\overline{E2}$)
$^{180}_{72}$Hf	501	-9.68×10^{-4} ($M2$)	-1.85×10^{-3} ($E3$)	-2.73×10^{-3} ($\overline{E2}$)
$^{182}_{74}$W	1189	-1.95×10^{-3} ($E1$)	-1.43×10^{-3} ($M2$)	-1.28×10^{-3} ($E3$)
		-1.65×10^{-3} ($\overline{E2}$)		
$^{183}_{74}$W	102.5	$+1.03\times10^{-2}$ ($M2$)	-1.21×10^{-2} ($\overline{E2}$)	
$^{187}_{75}$Re	72	-6.84×10^{-2} ($E1$)	-8.98×10^{-3} ($\overline{M1}$)	-7.70×10^{-3} ($\overline{E2}$)
$^{56}_{26}$Fe	2599	-1.18×10^{-4} ($M1$)	-1.08×10^{-4} ($E2$)	
	2015	-1.48×10^{-4} ($M1$)	-1.33×10^{-4} ($E2$)	
$^{95}_{41}$Nb	757	-8.71×10^{-4} ($M1$)	-7.39×10^{-4} ($E2$)	
	724	-8.99×10^{-4} ($M1$)	-7.61×10^{-4} ($E2$)	
$^{131}_{54}$Xe	364	-1.97×10^{-3} ($M1$)	-2.07×10^{-3} ($E2$)	
$^{133}_{54}$Xe	1298	-9.93×10^{-4} ($M1$)	-8.40×10^{-4} ($E2$)	
	530	-1.76×10^{-3} ($M1$)	-1.56×10^{-3} ($E2$)	
$^{133}_{55}$Cs	81	-2.78×10^{-3} ($M1$)	-1.29×10^{-2} ($E2$)	
$^{175}_{71}$Lu	396	-5.07×10^{-3} ($E1$)	-6.39×10^{-4} ($M2$)	
	283	-7.06×10^{-3} ($E1$)	$+1.50\times10^{-4}$ ($M2$)	
$^{189}_{76}$Os	147	-5.97×10^{-3} ($M1$)	-9.75×10^{-3} ($E2$)	
$^{192}_{55}$Pt	604	-3.57×10^{-3} ($M1$)	-2.76×10^{-3} ($E2$)	

and

$$\xi(\overline{E2})-\xi(E3)=-3.7\times10^{-4}\ ,$$

which are to be compared with the calculated ratio of PT- to P-violating matrix elements of 8×10^{-4}. Thus, it is possible to improve the limit set by the neutron electric dipole by a factor of at least 2 while still being above the sensitivity threshold for atomic final-state effects (still for the favorable isovector pion-exchange case).

Finally, we discuss the presence of final-state effects in experiments seeking to observe the presence of T-violating gamma-ray distributions. This causes the mixing ratio between multipoles with the same parity to acquire an imaginary phase. Taking, for example, $E2$ and $M1$ to be the competing multipoles, the experimentally observed T-violating quantity will be the imaginary part of the $M1$, $E2$ mixing ratio δ_{21}, which may be written as

$$\begin{aligned}\mathrm{Im}\delta_{21}=&\frac{\gamma(E2,a_0\to b)}{\gamma(M1,a_0\to b)}\\&\times\sum_z\left\{[\xi(E2)-\xi(M1)]\right.\\&+\left[\frac{\gamma(E2,a_z\to b)}{\gamma(E2,a_0\to b)}-\frac{\gamma(M1,a_z\to b)}{\gamma(M1,a_0\to b)}\right]\\&\left.\times\frac{\mathrm{Im}\langle a_z|V_T|a_0\rangle}{E_0-E_z}\right\}.\end{aligned}\tag{4}$$

Here the magnitude of the final-state effects relative to the true nuclear T violation is governed, in part, by the electromagnetic transition amplitudes unlike the PT violation, Eq. (3). Thus, as can be seen from Eq. (4), in pure T violation the comparative size of the atomic final-state effects may be significantly reduced by choosing nuclei for which the transitions admixed by V_T are much faster than the corresponding "regular" transitions, i.e., $\gamma(\pi L,a_z\to b)\gg\gamma(\pi L,a_0\to b)$. In the limiting case, where the "regular" transition is unmixed, the final-state effects can be made to disappear altogether. For example, if the "regular" transition is pure $M1$, i.e., $\gamma(E2,a_0\to b)=0$, then from Eq. (4) the $M1$, $E2$ mixing ratio is simply

$$\delta_{21}=\sum_z\frac{\gamma(E2,a_z\to b)}{\gamma(M1,a_0\to b)}\frac{\langle a_z|V_T|a_0\rangle}{E_0-E_z}\ ,\tag{5}$$

and contains no final-state phases. Since the right-hand side of Eq. (5) is pure imaginary, the T-violating phase angle attains its maximum value, $\sin\eta_{21}=\pm1$, and the inherent smallness of the T violation is reflected through $|\delta_{21}|$. (This example clearly shows that $|\delta|\cos\eta\sim1$ is not a condition ideally required of the observed gamma radiation [12]. Also, it should be noted that the true experimental measure of T violation is $|\delta|\sin\eta$ and not simply $\sin\eta$ as often quoted in the literature.) Thus, in principle, the atomic final-state phases need not place any restrictions on the experimental limits which can be set on possible T-violating effects.

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